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14. ABSTRACT

The present program aims to study the dynamics of droplet collision and flame-flow interaction that are of relevance to liquid-fueled turbulent combustion in propulsive devices. The investigation involves experimental, computational, and analytical components. The program recognizes the fundamental similarity between droplet collision and flame dynamics, especially from the computational viewpoint, in that both phenomena involve the tracking of deformable surfaces separating two media of vastly different densities. During the reporting period four classes of phenomena were investigated, namely: (1) The dynamics of binary droplet collision, especially on the criterion for the breaking of the inter-droplet surfaces which enables droplet merging. (2) The dynamics of droplet-film collision, especially on the influence of the film thickness in effecting droplet bouncing versus absorption. (3) The dynamics of droplet-droplet collision of dissimilar liquids, showing that the initiation of droplet internal superheating and hence microexplosion can be greatly facilitated by the presence of air bubbles entrained upon coalescence of the colliding droplets. (4) The dynamics and interaction of a freely propagating premixed flame with a vortex pair, with particular attention on the extent of flame wrinkling and flame-generated vorticity due to the generation of the baroclinic torque through the intrinsic hydrodynamic instability.

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Droplet collision; droplet-film collision; van der Waals force; droplet bouncing; droplet coalescence; microexplosion; flame-vortex interaction; hydrodynamic instability.

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DYNAMICS OF DROPLET COLLISION AND FLAME MOTION
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Introduction

The present program aims to study the dynamics of droplet collision and flame-flow interaction that are of relevance to liquid-fueled turbulent combustion in propulsive devices. The investigation involves experimental, computational, and analytical components. The program recognizes the fundamental similarity between droplet collision and flame dynamics, especially from the computational viewpoint, in that both phenomena involve the tracking of deformable surfaces separating two media of vastly different densities. Specifically, for droplet collision we are interested in the deformation of the droplet surface that separates the liquid and gas media, while for flame dynamics we are interested in the wrinkling of the flame front which separates the unburned and burned gas media.

During the reporting period four classes of phenomena were investigated, namely:

- (1) The dynamics of binary droplet collision, especially on the criterion for the breaking of the inter-droplet surfaces which enables droplet merging. The role of the van der Waals force in surface attraction is simulated.
- (2) The dynamics of droplet-film collision, especially on the influence of the film thickness in effecting droplet bouncing versus absorption, which is facilitated when the film thickness is comparable to the droplet diameter.
- (3) The dynamics of droplet-droplet collision of dissimilar liquids, showing that the initiation of droplet internal superheating and hence microexplosion can be greatly facilitated by the presence of air bubbles entrained upon coalescence of the colliding droplets.
- (4) The dynamics and interaction of a freely propagating premixed flame with a vortex pair, with particular attention on the extent of flame wrinkling and flame-

generated vorticity. Results based on the nature of the baroclinic torque generated through interaction demonstrate that, contrary to previous suggestions, hydrodynamic instability instead of vortex dynamics is the primary cause of the flame wrinkling. The computational descriptions of the above phenomena were enabled by: (5) The development of a numerical algorithm that accurately tracks the dynamics and geometry of immersed interfaces.

1. Dynamics of Binary Droplet Collision

Our previous studies on binary droplet collision revealed a non-monotonic outcome in terms of merging and bouncing as the collision intensity is varied. For the limiting situation of head-on collision, four regimes of distinctively different outcome with increasing collision Weber number (We) were experimentally observed. These four regimes are categorized according to: (I) permanent coalescence after minor droplet deformation, (II) bouncing, (III) permanent coalescence after substantial droplet deformation, and (IV) coalescence followed by separation and the concomitant production of daughter droplets. Clearly, it is of both fundamental and practical interest to be able to describe the transition boundaries between these regimes. While the transition between regimes III and IV has been successfully described, satisfactory quantitative descriptions have not been identified for the transitions between regimes I and II, and regimes II and III, hereafter referred to as transitions involving soft and hard collisions respectively. Phenomenologically, the propensity for bouncing or merging is a consequence of the readiness with which the gaseous mass in the inter-droplet gap can be squeezed out of the gap by the colliding interfaces such that they can make contact at the molecular level, leading to their destruction and thereby resulting in merging.

The lack of a clear criterion on the instant of surface rupture has also caused considerable uncertainty in the computational simulation of the collision event and consequently understanding of the collision and merging dynamics. Specifically, since the development of the shape and phase of the droplet deformation is driven through the interplay between the surface condition and the flow field, comparison between the global experimental and calculated collision images would allow the extraction of the detailed flow structure such as the contour and dynamics of the droplet surface and the

distributions of pressure, velocity, and energy budget. This information cannot be readily acquired experimentally due to the small dimension of the phenomena of interest, especially those within the inter-droplet gap. Furthermore, because of the richness of the phenomena involved, and because of the challenging need to track the displacement of a deformable, sharp interface, computational simulation of the experimental collision images can also serve to validate hydro-codes. However, since these hydro-codes are usually based on continuum mechanics, while the final stage of the interfacial dynamics leading to merging must necessarily involve rarified flows as well as molecular forces, the lack of such basic information renders it fundamentally impossible to simulate the interface rupture from first principles. This difficulty was circumvented by artificially, and quite arbitrarily, removing the interfaces at a certain instant when they are sufficiently close to each other. The fidelity of the simulation then depends on the instant at which rupture is implemented, especially it was found that the simulated dynamics depends very sensitively on this instant.

The present study was motivated by our experimental observation that the occurrence and instant of merging could be identified through a distinct change in the cuspy contour of the imaged interface, and the recognition that such an instant could be time resolved with sufficient accuracy such that, by using it as an input to the computational simulation based on continuum mechanics, the evolution of the experimental collision images subsequent to merging could be satisfactorily simulated.

Having established the adequacy of this empirically enabled computational simulation approach, we further studied the various issues related to the merging and bouncing aspects of the collision dynamics, including the energy budget, the flow field characteristics, and evolution of the geometry and dynamics of the inter-droplet gap, with emphasis on the transition between bouncing and merging regimes, and the differences between soft and hard collisions. The possible role of the van der Waals force in effecting merging was investigated, and the potential importance of compressibility and rarified gas effects for a complete description of the merging dynamics identified.

This work is reported in Publications [1, 2].

2. Dynamics of Droplet-Film Collision

In addition to droplet-droplet collision, droplet-surface collision is also of practical importance in the performance of spray-fueled combustors. That is, because of the droplet inertia acquired through spraying, it is well established that droplets can impinge onto the walls of the combustor. The occurrence of such events greatly modifies the gasification mode of the liquid fuel as well as the subsequent fuel vapor distribution. The influence is particularly significant in recognizing that the droplets that are most likely to impact the wall are the large ones, and that these large droplets contain substantial amount of the mass of the spray.

Based on our knowledge on droplet-droplet collision, it is reasonable to expect that the outcome of droplet-wall collision must fundamentally depend on two factors, namely whether the surface is dry or wet, and the thickness of the film when it is wet. Extensive experiments were conducted for the impingement of tetradecane droplets onto a brass surface, which is either dry or wet with controlled film thickness. Results showed that droplet-surface coalescence always occur when the surface is dry. When the surface is wet, the collision outcome depends sensitively on two parameters, namely the film thickness relative to the droplet radius, and the impact inertia characterized by the droplet Weber number. It was found that bouncing and coalescence are respectively favored for small and large We, which is reasonable. Furthermore, there exists a range in We over which merging is favored when the film thickness is of the order of the droplet diameter. Analytical study showed that this is caused by resonance induced by the natural frequency of oscillation as the droplet impacts the surface.

This work is reported in Ref. [3].

3. Micro-explosion of Collision-generated Droplets

Our studies on binary droplet collision has yielded an unexpected phenomenon that could have significant implications in understanding and optimizing spray combustion, namely the occurrence of mico-explosion of droplets of multicomponet fuels. To appreciate the relation between droplet collision and micro-explosion, we first note that multicomponent droplet combustion is of significant technical interest because most practical liquid fuels

are blends of many chemicals each characterized by its own physical-chemical properties, such as volatility, diffusivity, and reactivity. In particular, it is well established that the dominant factor governing the gasification of a multicomponent droplet is the exceedingly slow rate of liquid-phase mass diffusion relative to those of droplet surface regression and liquid-phase thermal diffusion. Consequently, as a droplet gasifies, the volatile components are initially preferentially gasified from the droplet surface, while the composition of the droplet interior remains practically unchanged. A concentration gradient is then set up within the droplet in such a manner that its composition changes from that of the interior, and hence initial, state to that of the surface which is more concentrated with the less volatile components. Since the less volatile components have higher boiling points, the droplet therefore sustains an equilibrium vaporization temperature higher than that based on the initial composition.

This diffusion-limited combustion mechanism has several implications. First, since gasification is initially dominated by the more volatile components, ignition of the droplet should also be affected more by the reactivity of these components. Second, since the droplet undergoes substantial heating as the less volatile components start to leave the droplet, the gasification rate of the droplet and hence the flame size should momentarily decrease during this transitional heating period. Third, after establishment of the concentration boundary layer, the droplet gasification rate should remain fairly steady. Fourth, the subsequent high surface and hence droplet temperature relative to the value for gasification of the interior implies that the droplet interior can potentially be heated to the limit of superheat. At this state, instantaneous internal gasification would take place, leading to violent rupturing, or micro-explosion, of the droplet. These unique characteristics of the combustion of a multicomponent droplet have been largely verified experimentally, although it has been noted that the occurrence of micro-explosion seems to depend on how the droplet was generated.

We next consider droplet collision. Our studies have shown that when two droplets impinge on each other, the pressure buildup in the inter-droplet space causes the otherwise convex droplet surfaces to become concave. Consequently the location of closest approach for the droplets is the rims forming the edge of the indentation. Thus a gas bubble would be entrained in the merged mass in the event that the droplets do merge

upon contact (at the rims). Furthermore, intense motion is generated within the interior of the merged mass upon coalescence, leading to dissipation of the excess surface energy and homogenization of the liquid's interior. Such motion could also disrupt the initially entrained gas bubble into smaller pieces. Thus the merged droplet could have one or more gas bubbles entrained in its interior. While the presence of the bubbles is not expected to affect a droplet's gasification and burning characteristics, they could initiate nucleation of the superheated liquid elements in the interior of the droplet. As such, it is possible that the merged droplet could micro-explode easier. The practical implication of such a possibility in enhanced atomization is quite apparent.

Two projects were undertaken to explore the phenomenon of collision-facilitated micro-explosion. The first project involved the collision between two droplets of high and low volatilities, respectively, such as heptane and hexadecane. Results conclusively demonstrated that while droplets of such a bi-component fuel do not micro-explode, they readily undergo micro-explosion when they were produced through collision. The second project involved the collision between an oil droplet and a water droplet. Because of the immiscible nature of water and oil, it was found that upon collision the water is usually embedded within hexadecane. Thus upon complete gasification of hexadecane which has a higher boiling point, the superheated water is exposed to the gaseous environment and flash vaporizes. In both cases the droplet lifetime is substantially reduced.

These works are respectively published in Refs. [4, 5].

4. The Role of Hydrodynamic Instability in Flame-Vortex Interaction

A useful elemental problem in the study of the structure of turbulent flames is that of flame-vortex interaction. In this approach, the interaction of a laminar flame with either an isolated vortex or a pair of vortices is viewed as a unit process of turbulent combustion in which the non-equilibrium zone of reaction and diffusion retains a locally laminar structure, and is treated as a wrinkled flame sheet. Extensive numerical studies have been undertaken to understand the ensuing interaction. In these studies constant density is sometimes assumed and the surface is simply treated as a passive one moving with a certain flame speed. In the lack of flame-flow coupling, stretch plays a key role in the kinematical behavior of the flame front. By allowing for thermal expansion across the

flame, earlier studies computationally showed that strain is not the only important parameter in characterizing flame-vortex interaction. Heat loss, curvature, viscous dissipation, and transient dynamics also have significant effects on the transition boundaries of the various turbulent flame regimes, especially for small-scale interactions. Furthermore, there exists a strong coupling between combustion heat release and fluid dynamics, and a significant amount of vorticity, which has the opposite sign to that of the initial vortex, is generated in the burned gas. These results were explained on the basis of the baroclinic torque generated by the density gradient across the flame and the pressure gradient of the initial vortex.

There were also some experimental investigations on flame–vortex interaction. Specifically, it was shown that significant amount of flame-generated vorticity (FGV) is present in the products immediately downstream of the flame. As such, FGV can be an important parameter affecting flame propagation and surface area production. The production source of FGV was attributed to the baroclinic torque generated by the density jump across the flame and the pressure gradients due to gravity and the initial vortex pair, and those induced by the flame curvature and variations in the burning velocity.

In this study we have computationally re-visited the interaction between a flame and a vortex pair, with particular interest in the role of hydrodynamic instability in flame wrinkling and vorticity generation. The study demonstrated that FGV is a natural outcome of the wrinkled flame for a weak vortical flow, with the baroclinic torque generated by the transverse pressure gradient along the wrinkled flame segment coupled with the density gradient across the flame. The initial non-uniform flow associated with the vortex therefore acts mostly as an initiation agent for the hydrodynamic instability experienced by the flame surface, with the pressure field of the vortex playing at most a minor role in the characteristics of the FGV. When the incoming vortex is strong enough, however, the combined influences of the imposed flow field and the hydrodynamic instability experienced by the flame characterize the subsequent vortex development.

This work was reported in Ref. [6].

5. An Immersed Boundary Method for Front Tracking

The computational phase of our studies on droplet collision and flame dynamics required the tracking of sharp interfaces. To meet this need a numerical algorithm was developed and is briefly described in the following.

Numerical simulation of flows with moving boundaries is relevant to a wide range of physical phenomena for which one needs to identify the shape, location, and movement of the interface in the course of computation. The problem is a challenging one, especially for situations in which properties change substantially across the interface, the interface geometry evolves drastically, and the front dynamics depends on the properties of the interface such as its curvature and variable gradient. A number of techniques, including those of Lagrangian, Eulerian, and mixed Eulerian-Lagrangian, have been developed. Prominent among them is the immersed-boundary method, which is based on the mixed Eulerian-Lagrangian approach, and incorporates interfacial conditions into the governing field equations by introducing additional source terms. Furthermore, while the interface thickness is zero in the context of continuum formulation, in the immersed-boundary method the condition defined at the supposedly sharp interface is numerically smeared out to the surrounding fixed grid points by locally weighted integration. To ensure that the computation strategy is fundamentally sound, overall conservation, such as that of mass, cannot be affected by the interface smearing. In addition, the jump conditions across the sharp interface must be satisfied globally, if not at the exact location of the interface.

The immersed-boundary method has been extensively applied to the study of drop and bubble dynamics, for which a key issue is the representation of surface tension by some suitable kernels. With surface tension smoothed out by the discrete δ -function and converted to a body force term, the governing equations can be solved for the entire domain without explicitly separating the different phases.

We have successfully adapted the immersed boundary method to our studies on droplet collision and flame dynamics, with further improvements on two issues, namely the unsteady pressure evolution and computation of the interface velocity.

This work is reported in Ref. [7].

Publications

1. "On the dynamics of head-on droplet collision: experiment and simulation," by K.L. Pan and C.K. Law, Paper No. AIAA 2004-1159, 42nd Aerospace sciences Meeting, Reno, NV, Jan. 5-8, 2004.
2. "Experimental and mechanistic descriptions of merging and bouncing in head-on binary droplet collision," by K.L. Pan, B. Zhou, and C.K. Law, submitted for publication.
3. "Dynamics of droplet-film collision," by K.L. Pan and C.K. Law, manuscript in preparation.
4. "On the burning and microexplosion of collision-generated bi-component droplets: miscible fuels," by C.H. Wang, W.G. Hung, S.Y. Fu, W.C. Huang, and C.K. Law, *Combustion and Flame*, Vol. 134, pp. 289-300 (2003).
5. "On the burning characteristics of collision-generated water/exadecane droplets," C.H. Wang, W.G. Hung, S.Y. Fu, W.C. Huang, and C.K. Law, *Combustion Science and Technology*, Vol. 176, No. 1, pp. 71-93 (2004).
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7. "An immersed boundary method for the dynamics of premixed flames," by K.L. Pan, W. Shyy, and C.K. Law, *International Journal of Heat and Mass Transfer*, Vol. 45, pp. 3503-3516 (2002).